LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049097.D
Acq On : 25 Jun 2021 19:22
Operator : CG/JU
Sample : M2829-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 15B-STOCKPILE-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049097.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.161	14	21	30	rBV2	52820	126100	6.13%	0.932%
2	3.232	30	33	39	rVB3	18361	31622	1.54%	0.234%
3	5.188	361	366	373	rBV	13533	23879	1.16%	0.177%
4	5.658	439	446	457	rBV	553768	929796	45.23%	6.874%
5	7.256	710	718	727	rBV	585620	1022623	49.75%	7.560%
6	8.108	853	863	868	rBV	141133	249020	12.11%	1.841%
7	9.272	1052	1061	1070	rBV	361115	664735	32.34%	4.914%
8	10.688	1294	1302	1313	rBV	233525	418605	20.36%	3.095%
9	10.923	1333	1342	1349	rBV	182411	338537	16.47%	2.503%
10	13.367	1750	1758	1767	rBV	899505	1401598	68.19%	10.362%
11	13.631	1798	1803	1812	rVB3	65598	105452	5.13%	0.780%
12	14.742	1983	1992	2000	rBV	273237	458579	22.31%	3.390%
13	15.682	2148	2152	2158	rVB4	19296	31308	1.52%	0.231%
14	16.163	2225	2234	2239	rBV4	21492	40417	1.97%	0.299%
15	16.234	2239	2246	2256	rVB	745535	1195612	58.17%	8.839%
16	17.491	2452	2460	2465	rBV	347275	544430	26.49%	4.025%
17	17.532	2465	2467	2478	rVV	75268	107247	5.22%	0.793%
18	17.621	2478	2482	2489	rVB2	16891	28866	1.40%	0.213%
19	18.149	2568	2572	2579	rVB	32942	50002	2.43%	0.370%
20	18.373	2604	2610	2614	rBV3	122760	180380	8.78%	1.334%
21	18.414	2614	2617	2621	rVB	20491	32163	1.56%	0.238%
22	18.561	2637	2642	2647	rBV3	25330	50222	2.44%	0.371%
23	18.666	2655	2660	2663	rBV6	15232	24941	1.21%	0.184%
24	19.225	2752	2755	2760	rBV5	14639	25607	1.25%	0.189%
25	19.283	2760	2765	2768	rBV6	28096	51415	2.50%	0.380%
26	19.313	2768	2770	2775	rVB3	75032	92787	4.51%	0.686%
27	19.448	2790	2793	2798	rVB2	33231	45027	2.19%	0.333%
28	19.542	2803	2809	2814	rVB	205532	301049	14.65%	2.226%
29	19.642	2822	2826	2831	rBV4	51669	72626	3.53%	0.537%
30	19.789	2847	2851	2859	rBV6	42806	67624	3.29%	0.500%
31	19.871	2860	2865	2867	rVV	54674	86923	4.23%	0.643%
32	19.906	2867	2871	2878	rVB	189658	285463	13.89%	2.110%
33	20.100	2897	2904	2909	rBV	1554379	2055544	100.00%	15.196%
34	20.218	2920	2924	2925	rBV3	17976	23185	1.13%	0.171%
35	20.364	2945	2949	2951	rBV5	35180	47011	2.29%	0.348%
36	20.394	2952	2954	2958	rVB2	52108	63316	3.08%	0.468%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049097.D
Acq On : 25 Jun 2021 19:22
Operator : CG/JU
Sample : M2829-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 15B-STOCKPILE-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.494	2967	2971	2974	rBV3	24591	38891	1.89%	0.288%
38	20.547	2976	2980	2986	rVV4	23422	49637	2.41%	0.367%
39	20.729	3008	3011	3016	rVB3	37134	48290	2.35%	0.357%
40	20.829	3025	3028	3036	rBV9	19812	42899	2.09%	0.317%
41	21.404	3122	3126	3130	rBV3	94266	146604	7.13%	1.084%
42	21.780	3181	3190	3195	rBV3	344534	792198	38.54%	5.857%
43	21.822	3195	3197	3205	rVB	91532	140576	6.84%	1.039%
44	21.980	3219	3224	3228	rBV5	25483	53647	2.61%	0.397%
45	24.043	3569	3575	3582	rBV2	70500	200318	9.75%	1.481%
46	24.777	3698	3700	3701	rBV2	24601	20706	1.01%	0.153%
47	24.941	3721	3728	3736	rVB2	63198	161614	7.86%	1.195%
48	25.094	3746	3754	3765	rBV2	185537	557592	27.13%	4.122%

Sum of corrected areas: 13526683

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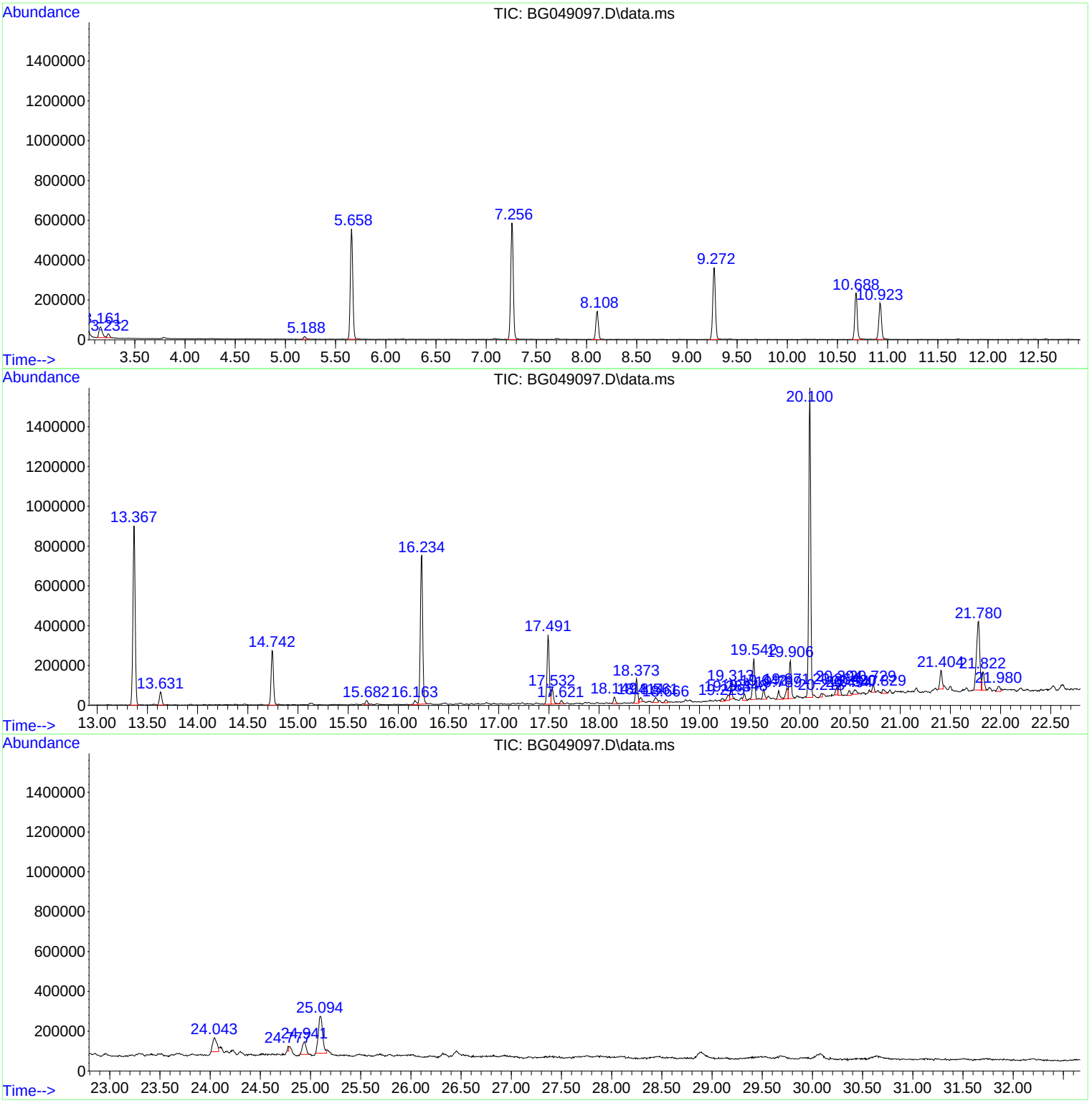
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
15B-STOCKPILE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049097.D
Acq On : 25 Jun 2021 19:22
Operator : CG/JU
Sample : M2829-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
15B-STOCKPILE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

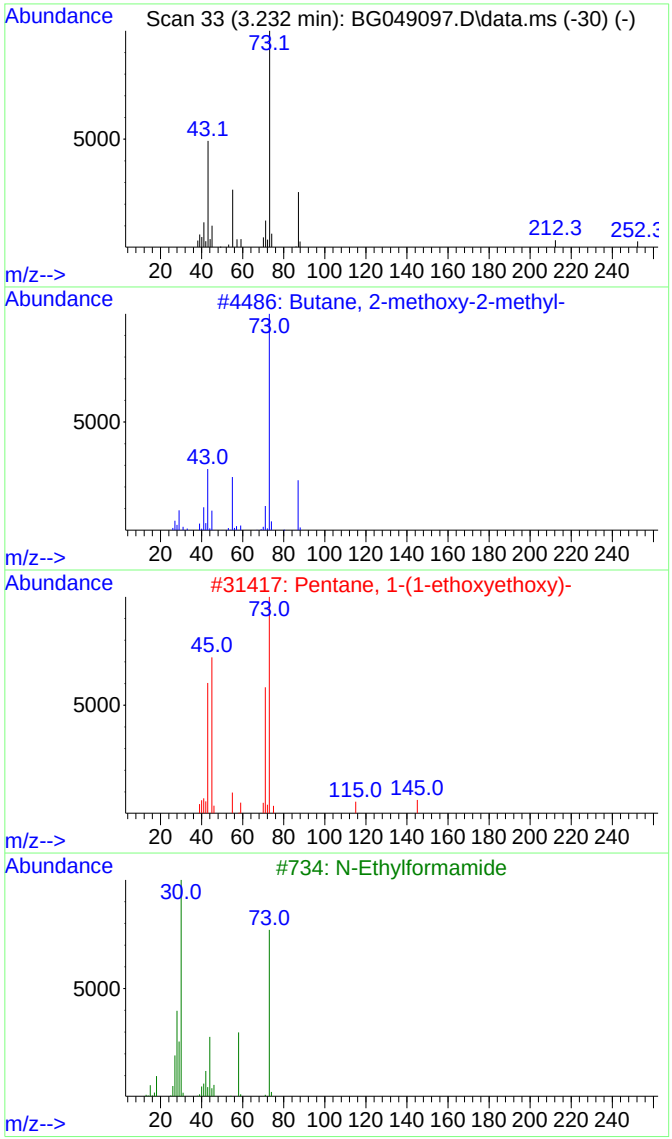
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

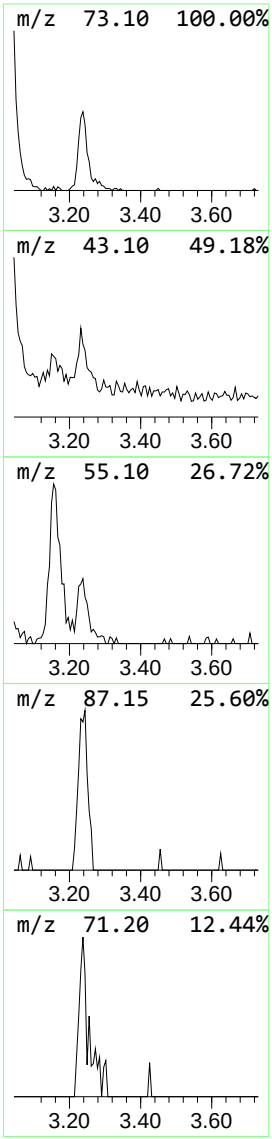
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.232	2.54 ng	31622	1,4-Dichlorobenzene-d4	8.108

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Pentane, 1-(1-ethoxyethoxy)-	160	C9H20O2	013442-89-2	10
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049097.D
Acq On : 25 Jun 2021 19:22
Operator : CG/JU
Sample : M2829-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 15B-STOCKPILE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

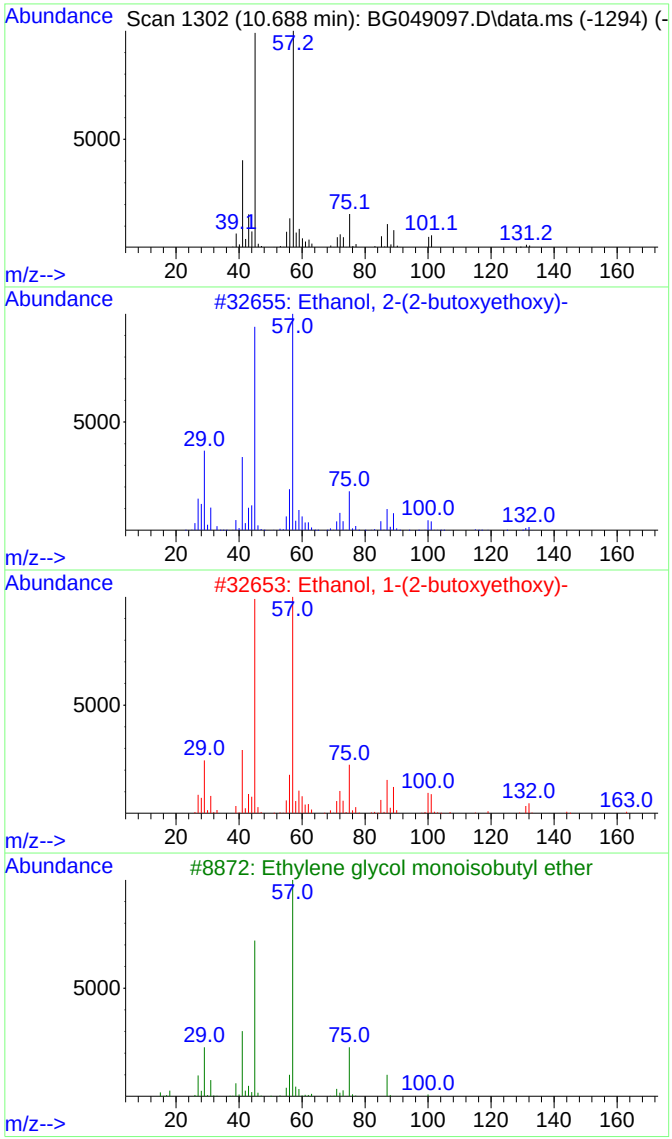
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

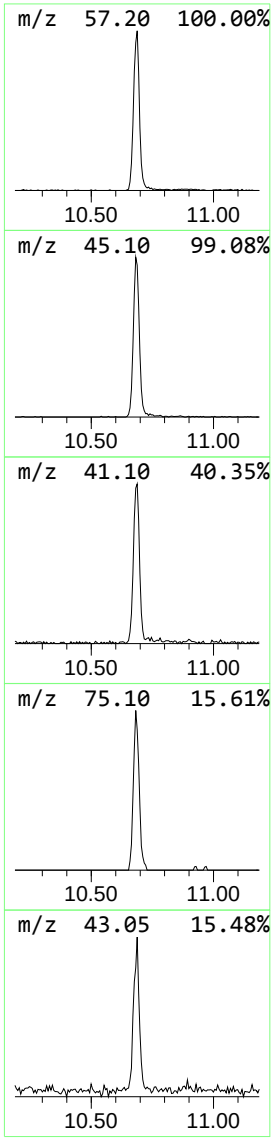
****

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.688	24.73 ng	418605	Naphthalene-d8	10.923

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	Di-sec-butyl ether	130	C8H18O	006863-58-7	59
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049097.D
Acq On : 25 Jun 2021 19:22
Operator : CG/JU
Sample : M2829-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
15B-STOCKPILE-1

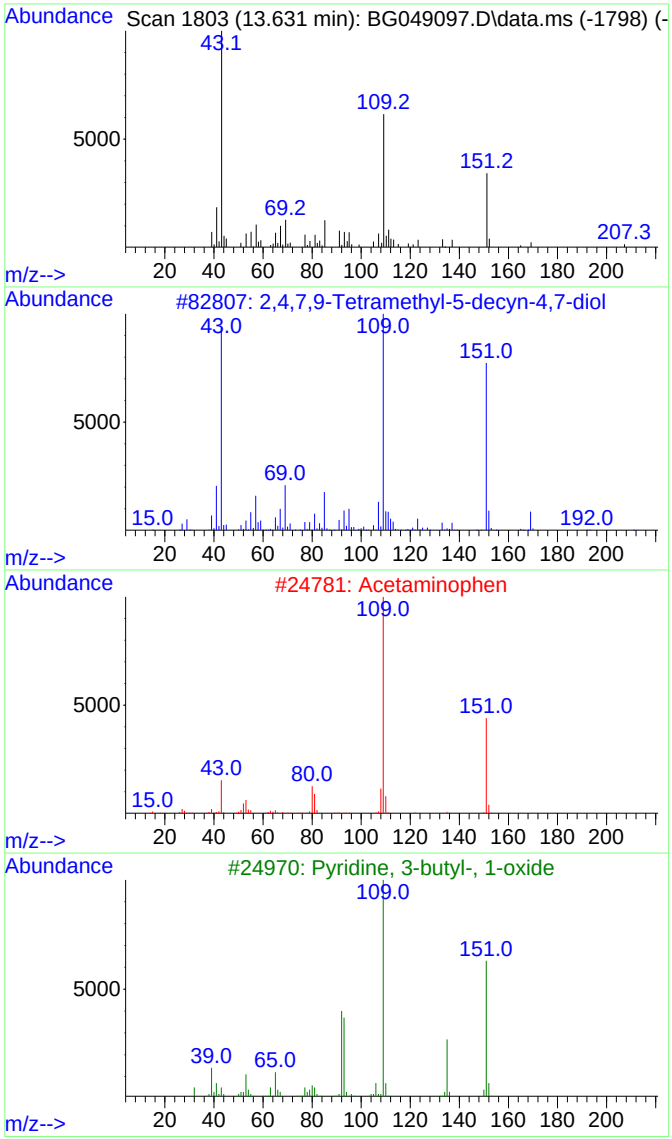
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

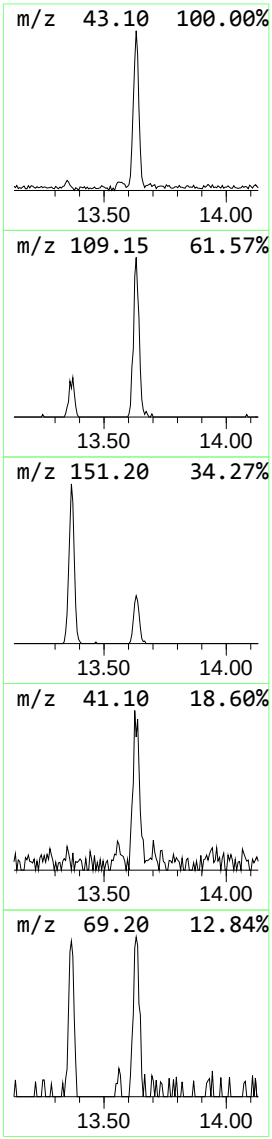
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.631	4.60 ng	105452	Acenaphthene-d10	14.742

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90
2	Acetaminophen	151	C8H9NO2	000103-90-2	49
3	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	49
4	Metacetamol	151	C8H9NO2	000621-42-1	49
5	Benzenamine, 4-propoxy-	151	C9H13NO	004469-80-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049097.D
Acq On : 25 Jun 2021 19:22
Operator : CG/JU
Sample : M2829-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 15B-STOCKPILE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

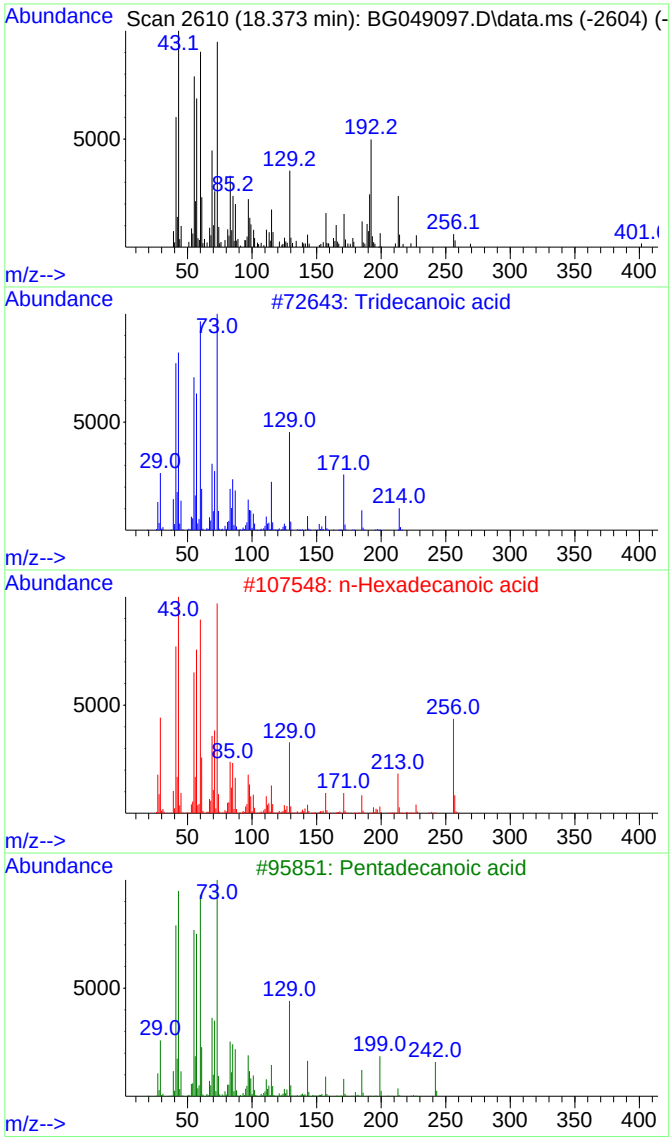
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

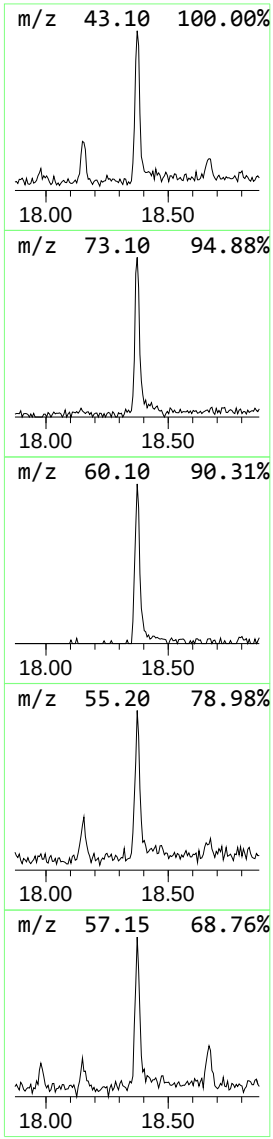
****

Peak Number 5 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.373	6.63 ng	180380	Phenanthrene-d10	17.491

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049097.D
Acq On : 25 Jun 2021 19:22
Operator : CG/JU
Sample : M2829-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
15B-STOCKPILE-1

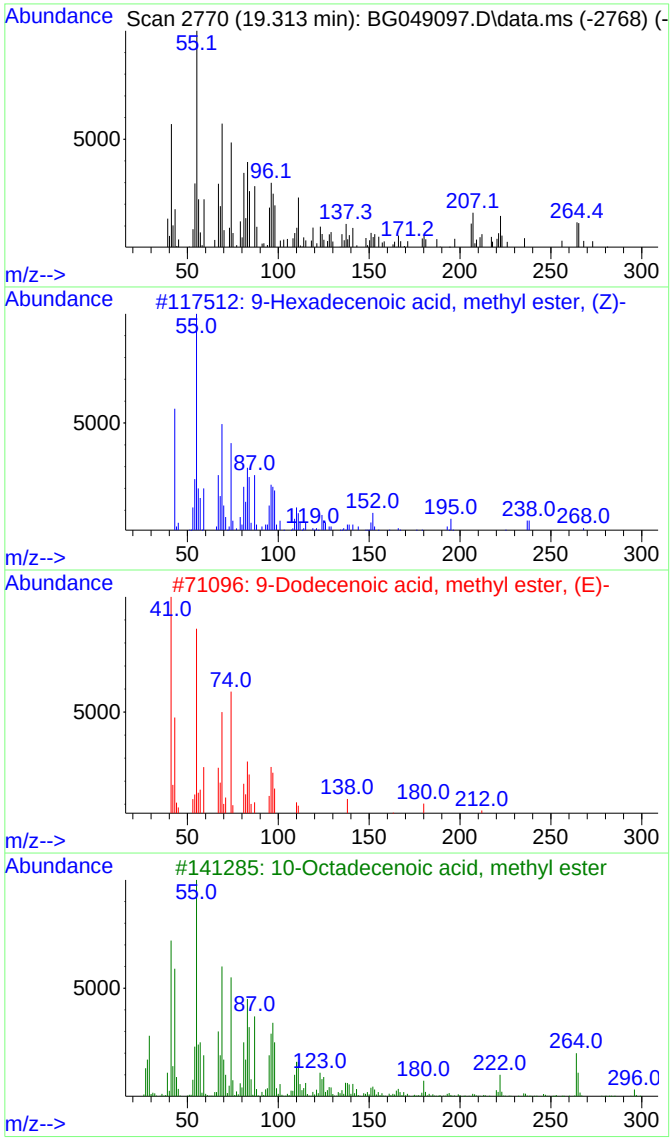
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

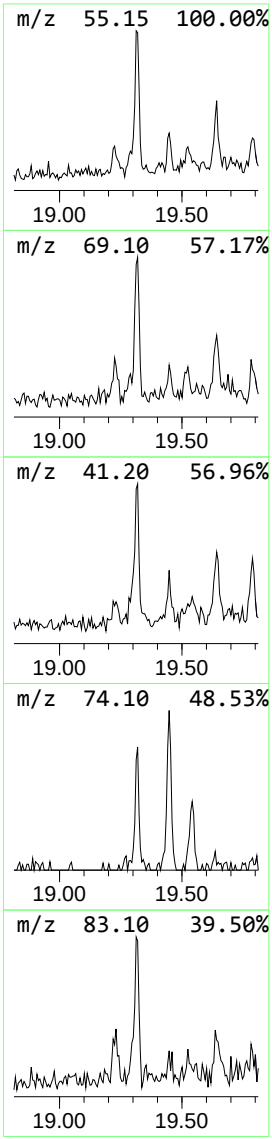
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9-Hexadecenoic acid, methyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.313	3.41 ng	92787	Phenanthrene-d10	17.491

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	91
2	9-Dodecenoic acid, methyl ester,...	212	C13H24O2	055030-26-7	70
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	64
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	64
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	62





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Data File : BG049097.D
Acq On : 25 Jun 2021 19:22
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Sample : M2829-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
15B-STOCKPILE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

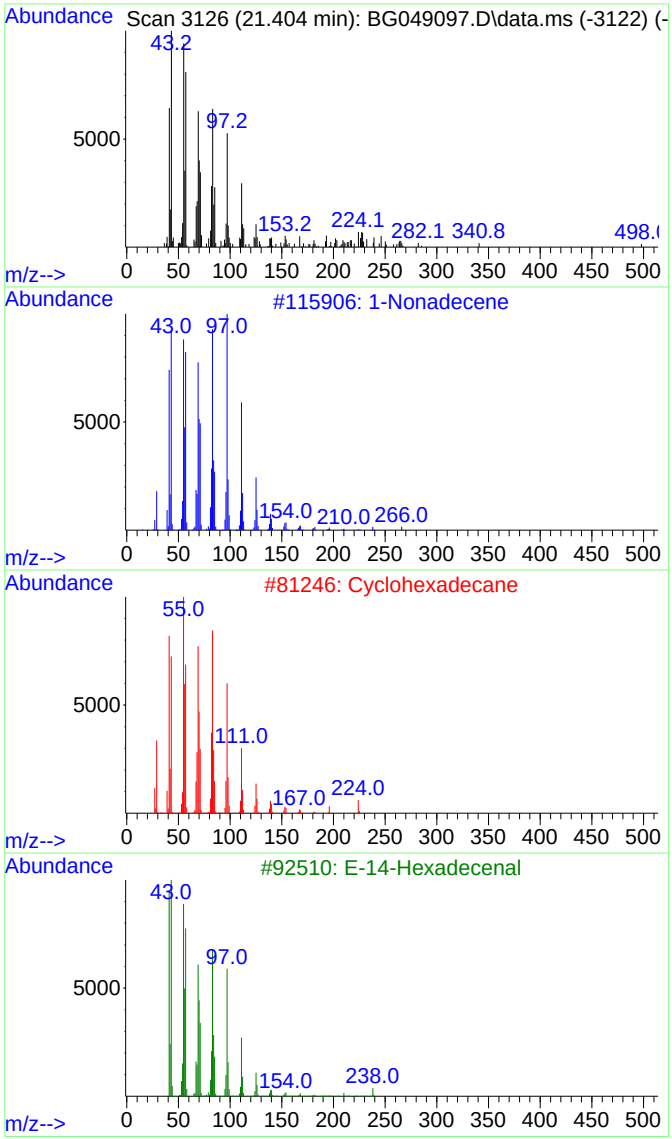
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

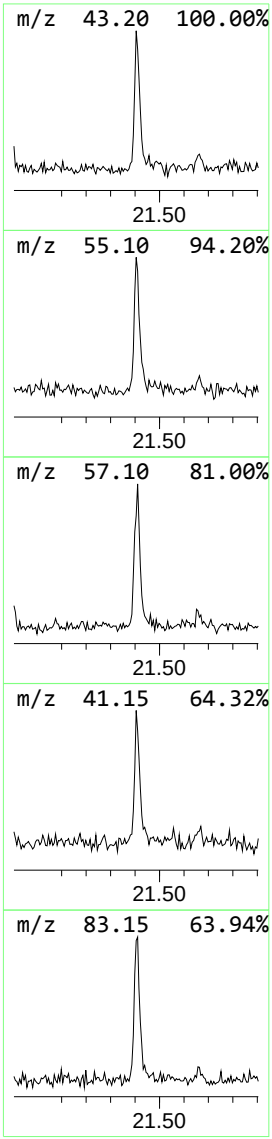
****

Peak Number 7 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.404	3.70 ng	146604	Chrysene-d12	21.780

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	98
2	Cyclohexadecane	224	C16H32	000295-65-8	94
3	E-14-Hexadecenal	238	C16H30O	330207-53-9	94
4	1-Pentadecanethiol	244	C15H32S	025276-70-4	92
5	9-Nonadecene	266	C19H38	031035-07-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062521\
Data File : BG049097.D
Acq On : 25 Jun 2021 19:22
Operator : CG/JU
Sample : M2829-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 15B-STOCKPILE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.232	2.5	ng	31622	1	8.108	249020	20.0
Ethanol, 2-(2-b...	10.688	24.7	ng	418605	2	10.923	338537	20.0
2,4,7,9-Tetrame...	13.631	4.6	ng	105452	3	14.742	458579	20.0
Tridecanoic acid	18.373	6.6	ng	180380	4	17.491	544430	20.0
9-Hexadecenoic ...	19.313	3.4	ng	92787	4	17.491	544430	20.0
1-Nonadecene	21.404	3.7	ng	146604	5	21.780	792198	20.0